A Generalized Non-Equilibrium Bounce-Back Condition for Multi-Component DdQn Lattice Boltzmann Models with Wetting Applications.

D. Schrijver

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Abstract will come here…

I. INTRODUCTION

Introduction will come here…

II. KNUDSEN EXPANSION

In diffusive scaling, we get the following for a Knudsen expansion,

$$\begin{aligned} f_i^{(0)} &= f_i^{\mathrm{eq},(0)} = w_i\rho^{(0)}, \\ f_i^{(1)} &= f_i^{\mathrm{eq},(1)} = w_i\rho^{(1)} + w_i\rho^{(0)}\frac{\boldsymbol{u}^{(1)}\cdot\boldsymbol{c}_i}{c_s^2}, \\ f_i^{(2)} &= f_i^{\mathrm{eq},(2)} - \frac{\tau}{Sh}\left(c_{i\alpha}\partial_\alpha f_i^{\mathrm{eq},(1)}\right). \end{aligned} \tag{1}$$

This gives the non-equilibrium part up to second order in Knudsen number,

$$\begin{aligned} f_i^{\mathrm{neq}} = -\frac{\tau}{Sh}\left(\partial_\alpha\left(w_i c_{i\alpha}\rho^{(1)}\right) + \frac{\rho^{(0)}}{c_s^2}\partial_\alpha\left(w_i c_{i\alpha}c_{i\beta}u_\beta\right)\right) \\ + \mathcal{O}\left(Kn^3\right). \end{aligned} \tag{2}$$

We now want to plug this into the equation for the NEBB boundary condition,

$$\begin{aligned} f_i^{\mathrm{neq}} &= f_q^{\mathrm{neq}} - \sum_\alpha w_i c_{i\alpha} N_\alpha, \\ N_\alpha &= \frac{1}{\sum_i^{\mathrm{in}} w_i c_{i\alpha}^2}\sum_i^{\mathrm{par}} f_i c_{i\alpha} \equiv C_\alpha \sum_i^{\mathrm{par}} f_i c_{i\alpha}. \end{aligned} \tag{3}$$

We now want to add stress corrections,

$$f_i^{\mathrm{neq}} = f_q^{\mathrm{neq}} - \sum_\alpha w_i c_{i\alpha}N_\alpha - \sum_\mu\sum_\nu w_i c_{i\mu}c_{i\nu}M_{\mu\nu} \tag{4}$$

The corrections can be found using the expected Navier-Stokes second moment,

$$\Pi_{\alpha\beta}^{\mathrm{NS}} = -\tau c_s^2\rho\left(\partial_\alpha u_\beta + \partial_\beta u_\alpha\right) \tag{5}$$

The velocity gradients can be estimated using finite differences. We now want to ensure the following,

$$\sum_i c_{i\alpha}c_{i\beta}f_i = \Pi_{\alpha\beta}^{\mathrm{NS}}. \tag{6}$$

This gives the following tensor equation,

$$\sum_\mu\sum_\nu Q_{\alpha\beta\mu\nu}M_{\mu\nu} = B_{\alpha\beta} \tag{7}$$

With the following definitions,

$$\begin{aligned} Q_{\alpha\beta\mu\nu} &\equiv -\sum_i^{\mathrm{in}} w_i c_{i\alpha}c_{i\beta}c_{i\mu}c_{i\nu}, \\ B_{\alpha\beta} &\equiv \Pi_{\alpha\beta}^{\mathrm{NS}} - A_{\alpha\beta}, \\ A_{\alpha\beta} &\equiv 2\sum_i^{\mathrm{out}} c_{i\alpha}c_{i\beta}f_i + \sum_i^{\mathrm{par}} c_{i\alpha}c_{i\beta}f_i \\ &\quad + \sum_i^{\mathrm{in}} c_{i\alpha}c_{i\beta}\left(2w_i\rho\frac{\boldsymbol{u}\cdot\boldsymbol{c}_i}{c_s^2} - \sum_\gamma w_i c_{i\gamma}N_\gamma\right). \end{aligned} \tag{8}$$

For a boundary in the yz, xz and xy-planes, Eq. (7) can be solved if we use the D3Q27 stencil,

$$\underline{\underline{M}} = \begin{pmatrix} -12B_{00}+9B_{11}+9B_{22} & -18B_{01} & -18B_{02} \\ -18B_{01} & 9B_{00}-27B_{11} & -54B_{12} \\ -18B_{02} & -54B_{12} & 9B_{00}-27B_{22} \end{pmatrix} \tag{9}$$

$$\underline{\underline{M}} = \begin{pmatrix} -27B_{00}+9B_{11} & -18B_{01} & -54B_{02} \\ -18B_{01} & 9B_{00}-12B_{11}+9B_{22} & -18B_{12} \\ -54B_{02} & -18B_{12} & 9B_{11}-27B_{22} \end{pmatrix} \tag{10}$$

$$\underline{\underline{M}} = \begin{pmatrix} -27B_{00}+9B_{22} & -54B_{01} & -18B_{02} \\ -54B_{01} & -27B_{11}+9B_{22} & -18B_{12} \\ -18B_{02} & -18B_{12} & 9B_{00}+9B_{11}-12B_{22} \end{pmatrix} \tag{11}$$